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Claims

1. A method for the production of an organic molecule having a desired property, comprising the steps of:

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(a) providing a starting group of different organic molecules;

(b) causing at least one chemical reaction to take place with at least some of the different organic molecules in the starting group to create an intermediate reaction mixture having one or more organic molecules different from the organic molecules in the starting group;

10 (c) repeating step (b) at least once by substituting the intermediate reaction mixture as the starting group to thereby produce a final reaction mixture as a result of the last repetition; and

15 (d) screening the final reaction mixture resulting from step (c) for the presence of the organic molecule having the desired property.

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2. The method of claim 1 further comprising the step of isolating from the final reaction mixture the organic molecule having the desired property.

3. The method of claim 1 further comprising the step of determining the structure or functional properties characterizing the organic molecule having the desired property.

4. The method of claim 3 further comprising the step of synthesizing the organic molecule having the desired property.

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5. The method of claim 1 further comprising the step of adding more of the starting group of different organic molecules to the intermediate reaction mixture after at least one repetition of step (b).

5 6. The method of claim 1 wherein the different organic molecules of the starting group all share a common core structure.

10 7. The method of claim 1 wherein the different organic molecules of the starting group are selected from the group consisting of alkanes, alkenes, alkynes, arenes, alcohols, ethers, amines, aldehydes, ketones, acids, esters, amides, cyclic compounds, heterocyclic compounds, organometallic compounds, hetero-atom bearing compounds, amino acids, nucleotides, and mixtures thereof.

15 8. The method of claim 7 wherein the different organic molecules of the starting group are selected from the group consisting of acids, amines, alcohols, amino acids, nucleotides, and unsaturated compounds.

9. The method of claim 8 wherein the different organic molecules of the starting group are selected from the group consisting of amino acids and nucleotides.

20 *Sub D2* 10. The method of claim 1 wherein the at least one chemical reaction for each repetition of step (b) is independently selected from the group consisting of substitution, addition, elimination, rearrangement, dehydration, reduction, oxidation, condensation, hydrogenation, dehydrogenation, dimerization, epoxidation, isomerization, cyclization, decyclization, halogenation, sulfonation, alkylation, acylation, nitration, hydrolysis, esterification, transesterification, carboxylation, decarboxylation, amination, and deamination.

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11. The method of claim 1 wherein the chemical reaction is caused by changing the conditions of the intermediate reaction mixture, by taking a step selected from the group consisting of adding water, removing water, adding air, adding oxygen, adding ammonia, changing 5 temperature, changing pressure, adding an oxidizing agent, adding a reducing agent, adding a source of radiation, adding a hydroxylating agent, adding a hydrogenating agent, adding a dehydrogenating agent, adding an epoxidizing agent, adding a halogenating agent, adding a sulfonating agent, adding an alkylating agent, adding an acylating agent, 10 adding a nitrating agent, adding a hydrolytic agent, adding a carboxylating agent, adding a decarboxylating agent, changing concentration, adding a new solvent, changing pH, and adding a catalyst.

12. The method of claim 1 wherein the at least one chemical 15 reaction is caused by adding a set of different enzymes.

13. The method of claim 12 wherein at least 10,000 different enzymes are added.

14. The method of claim 13 wherein at least 1,000,000 different enzymes are added.

20 15. The method of claim 14 wherein at least 100,000,000 different enzymes are added.

16. The method of claim 1 wherein the conditions causing the chemical reactions of steps (b) and (c) are the same.

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17. The method of claim 1 further comprising the step of using a selection method on the intermediate reaction mixture to produce a subset of organic molecules with a higher likelihood of producing the organic molecule having the desired property.

5 18. The method of claim 17 wherein the selection method comprises using a chemostat.

10 19. The method of claim 1 wherein at least one agent, selected from the group consisting of oxidizing agents, reducing agents, hydrating agents, dehydrating agents, hydroxylating agents, hydrogenating agents, dehydrogenating agents, epoxidizing agents, halogenating agents, sulfonating agents, alkylating agents, acylating agents, nitrating agents, hydrolytic agents, carboxylating agents, and decarboxylating agents, is added during at least one repetition of step (b).

15 20. The method of either claim 1 or claim 7 wherein the starting group contains at least 10 different organic molecules.

21. The method of claim 20 wherein the starting group contains at least 100 different organic molecules.

20 22. The method of claim 21 wherein the starting group contains at least 1,000 different organic molecules.

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23. A method for the production of an organic molecule having a desired property, comprising the steps of:

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10 (a) providing a starting group of different organic molecules;

15 (b) causing at least one chemical reaction to take place with at least some of the different organic molecules in the starting group to create an intermediate reaction mixture having one or more organic molecules different from the organic molecules in the starting group;

20 (c) repeating step (b) at least once by substituting the intermediate reaction mixture as the starting group to thereby produce a final reaction mixture as a result of the last repetition;

25 (d) screening the final reaction mixture resulting from step (c) for the presence of the organic molecule having the desired property; and

30 (e) if the organic molecule is found in the final reaction mixture, then performing the following additional steps:

(1) dividing the starting group of different organic molecules into at least two subgroups, each containing less than all of the different organic molecules in the starting group;

(2) performing steps (b) and (c) on each of the subgroups in the same way as performed with the starting group to produce a final reaction submixture corresponding to each of the subgroups;

(3) screening each of the final reaction submixtures resulting from step (2) for the presence of the organic molecule having the desired property; and

(4) repeating at least once, steps (1) through (3) for at least one of the successful subgroups from which the organic molecule having the desired property is produced,

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by substituting the successful subgroup as the subgroup in step (1) to thereby identify a narrowed group of different organic molecules from which the compound having the desired property can be produced.

5 24. A method for the production of an organic molecule having a desired property, comprising the steps of:

10 (a) providing a starting group of different organic molecules;

15 (b) causing at least one chemical reaction to take place with at least some of the different organic molecules in the starting group to create an intermediate reaction mixture having one or more organic molecules different from the organic molecules in the starting group;

20 (c) repeating step (b) at least once by substituting the intermediate reaction mixture as the starting group to thereby produce a final reaction mixture as a result of the last repetition;

25 (d) screening the final reaction mixture resulting from step (c) for the presence of the organic molecule having the desired property; and

30 (e) if the organic molecule having the desired property is found in the final reaction mixture, then performing the following additional steps:

 (1) providing at least two additional starting groups of different organic molecules, each additional starting group corresponding to the starting group of step (a);

 (2) performing steps (b) and (c) on each of the additional starting groups in the same way as performed with the starting group of step (a) with the exception that, for each of the additional starting groups, at least one of

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the chemical reactions is eliminated to thereby produce an additional final reaction mixture from each of the additional starting groups;

(3) screening each of the additional final reaction mixtures resulting from step (2) for the presence of the organic molecule having the desired property;

10 (4) repeating, at least once, steps (1) through (3) for at least one of the successful additional starting groups from which the organic molecule having the desired property is produced, by substituting the successful additional starting group as the additional starting group in step (1) to thereby identify a narrowed group of chemical reactions from which the compound having the desired property can be produced.

15 25. A method for the production of an organic molecule having a desired property, comprising the steps of:

20 (a) providing a starting group of at least 100 different organic molecules selected from the group consisting of alkanes, alkenes, alkynes, arenes, alcohols, ethers, amines, aldehydes, ketones, acids, esters, amides, cyclic compounds, heterocyclic compounds, organometallic compounds, hetero-atom bearing compounds, amino acids, nucleotides, and mixtures thereof;

25 (b) causing at least one chemical reaction selected from the group consisting of substitution, addition, elimination, rearrangement, dehydration, reduction, oxidation, condensation, hydrogenation, dehydrogenation, dimerization, epoxidation, isomerization, cyclization, decyclization, halogenation, sulfonation, alkylation, acylation, nitration, hydrolysis, esterification, transesterification, carboxylation, decarboxylation, amination, and deamination to take place with at least some of the different

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organic molecules in the starting group to create an intermediate reaction mixture having one or more organic molecules different from the organic molecules in the starting group;

5 (c) repeating step (b) at least once by substituting the intermediate reaction mixture as the starting group to thereby produce a final reaction mixture as a result of the last repetition;

10 (d) screening the final reaction mixture resulting from step (c) for the presence of the organic molecule having the desired property;

(e) isolating from the final reaction mixture the organic molecule having the desired property; and

(f) determining the structure or functional properties characterizing the organic molecule having the desired property.

15 26. The method of claim 25 wherein the different organic molecules of the starting group all share a common core structure.

20 *Sub DS* 27. The method of claim 26 further comprising the step of using a selection method on the intermediate reaction mixture to produce a subset of organic molecules with a higher likelihood of producing the organic molecule having the desired property.

28. The method of claim 27 wherein the at least one chemical reaction is caused by adding a set of different enzymes.

29. A method for the production of an organic molecule having a desired property, comprising the steps of:

25 (a) reacting a group of different substrates, the group comprising acids, amines, alcohols, and unsaturated compounds, under suitable conditions with a dehydrating agent to yield a first reaction mixture;

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- (b) reacting the first reaction mixture with a reducing agent under suitable conditions to yield a second reaction mixture;
- 5 (c) reacting the second reaction mixture with an oxidizing agent under suitable conditions to yield a third reaction mixture;
- (d) performing a condensation reaction under suitable conditions upon the third reaction mixture to yield a fourth reaction mixture;
- 10 (e) exposing the fourth reaction mixture to light with a wavelength of about 220 nanometers to 600 nanometers, thereby producing one or more organic molecules different from the substrates and agents;
- 15 (f) screening the exposed fourth reaction mixture for the presence of the organic molecule having the desired property; and
- (g) isolating from the exposed fourth reaction mixture the organic molecule having the desired property.

30. A method of generating for characterization an organic molecule having a desired property, comprising the steps of:

- 20 (a) reacting a group of different substrates, the group comprising acids, amines, alcohols, and unsaturated compounds, under suitable conditions with a dehydrating agent to yield a first reaction mixture;
- , 25 (b) reacting the first reaction mixture with a reducing agent under suitable conditions to yield a second reaction mixture;
- 30 (c) reacting the second reaction mixture with an oxidizing agent under suitable conditions to yield a third reaction mixture;

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(d) performing a condensation reaction under suitable conditions upon the third reaction mixture to yield a fourth reaction mixture;

5 (e) exposing the fourth reaction mixture to light with a wavelength of about 220 nanometers to 600 nanometers, thereby producing one or more organic molecules different from the substrates and agents;

10 (f) screening the exposed fourth reaction mixture for the presence of the organic molecule having the desired property; and

(g) determining the structure or functional properties characterizing the organic molecule having the desired property.

31. The method of claim 30, additionally including, prior to step (g), isolating from the reaction mixture the organic molecule having the desired property.

15 32. The method of either claim 29 or claim 30, additionally including, prior to step (f), repeating steps (a)-(e) with or without introducing additional substrates.

20 33. The method of either claim 29 or claim 30 wherein the order in which the substrates are subjected to the reactions of steps (a)-(e) is varied.

34. The method of either claim 29 or claim 30, further including after step (g), producing the organic molecule having the desired property.

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35. The method of either claim 29 or claim 30 wherein the desired property is the ability to function as a drug, a vaccine, a ligand, a catalyst, a catalytic cofactor, a structure of use, a detector molecule, or a building block for another compound.

5 36. A method for the production of an organic molecule having a desired property, comprising the steps of:

10 (a) reacting a group of different enzymes representing a diversity of catalytic activities under suitable conditions with a group of different substrates to create a reaction mixture, thereby producing one or more organic molecules different from the enzymes and substrates in the reaction mixture;

15 (b) screening the reaction mixture for the presence of the organic molecule having the desired property; and

15 (c) isolating from the reaction mixture the organic molecule having the desired property.

37. A method of generating for characterization an organic molecule having a desired property, comprising the steps of:

20 (a) reacting a group of different enzymes representing a diversity of catalytic activities under suitable conditions with a group of different substrates to create a reaction mixture, thereby producing one or more organic molecules different from the enzymes and substrates in the reaction mixture;

25 (b) screening the reaction mixture for the presence of the organic molecule having the desired property; and

25 (c) determining the structure or functional properties characterizing the organic molecule having the desired property.

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38. The method of claim 37, additionally including, prior to step (c), isolating from the reaction mixture the organic molecule having the desired property.

5 39. The method of either claim 36 or claim 37 wherein the group of different substrates is selected from the group consisting of alkanes, alkenes, alkynes, arenes, alcohols, ethers, amines, aldehydes, ketones, acids, esters, amides, cyclic compounds, heterocyclic compounds, organometallic compounds, hetero-atom bearing compounds, amino acids, nucleotides, and mixtures thereof.

10 40. The method of claim 39 wherein the group of different substrates is selected from the group consisting of acids, amines, alcohols, amino acids, nucleotides, and unsaturated compounds.

15 41. The method of claim 40 wherein the group of different substrates is selected from the group consisting of amino acids and nucleotides.

42. The method of claim 39 wherein the group of different substrates contains at least 100 different organic molecules.

43. The method of claim 42 wherein the group of different substrates contains at least 1,000 different organic molecules.

20 44. The method of either claim 36 or claim 37, further comprising after step (c), producing the organic molecule having the desired property.

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45. The method of either claim 36 or claim 37, wherein the desired property is the ability to function as a drug, a vaccine, a ligand, a catalyst, a catalytic cofactor, a structure of use, a detector molecule, or a building block for another compound.

5 46. The method of either claim 36 or claim 37 wherein the group of different enzymes comprises at least 10,000 different enzymes.

47. The method of claim 46 wherein the group of different enzymes comprises at least 1,000,000 different enzymes.

10 48. The method of claim 47 wherein the group of different enzymes comprises at least 100,000,000 different enzymes.

49. The method of either claim 36 or claim 37, wherein the substrates of the group of different substrates all share a common core structure.

15 50. The method of either claim 36 or claim 37, further comprising the step of using a selection method on the reaction mixture to produce a subset of organic molecules with a higher likelihood of producing the organic molecule having the desired property.